

SEPARATING THE VARIANCES OF A TWO-COMPONENT CLOCK MODEL BY SEQUENTIAL MINQUE

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Abstract

Minimum norm quadratic unbiased estimation, or MINQUE, is a method for improving the variance estimates of noise components in a Gauss-Markov least-squares problem. This study treats a simple special case: estimating the two noise levels of a clock whose phase noise is the sum of white FM and random walk FM. Given prior estimates of the noise levels, perhaps from an Allan deviation plot, MINQUE calculates new estimates and their uncertainties. Although the original MINQUE calculation on N data takes $O(N^2)$ space and $O(N^3)$ time, it can be done sequentially in bounded space and $O(N)$ time. The method is applied to data from a simulation and from a comparison of two hydrogen masers.

INTRODUCTION

Having observed time deviations (or “phase”) $x(t)$ of a clock or pair of clocks, one may wish to fit the noise levels h_α of a power-law spectral model, $S_y(f) = \sum_{\alpha=-2}^2 h_\alpha f^\alpha$, where $y = dx/dt$. This is often done graphically by identifying regions of constant slope on log-log plots of frequency stability deviations, including Allan deviation, Hadamard deviation, and their modified forms that use interval averages \bar{x} instead of point values $x(t)$. Objective statistical procedures for estimating the h_α and their uncertainties have been devised. Tryon and Jones [1] estimated the noise levels of an ensemble of several cesium clocks by maximizing the likelihood function of the residuals of a Kalman filter operating on the clock differences. In the “multivariate” methods, the data consist of estimates of several different frequency stability variances at a set of averaging times: Vernotte *et al.* [2] estimated the noise levels by a weighted least-squares technique; Walter [3] estimated the noise levels and mean frequency drift rate by minimizing a cost function composed of certain chi-squared statistics.

The present paper is an initial effort to exploit a general method of noise level estimation, called minimum norm quadratic unbiased estimation, or MINQUE, invented by the statistician C. R. Rao [4]. This is a method for improving the estimates of noise levels in a linear model $z = Xb + \varepsilon$, where z is a

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vector of observations, X is a known matrix, b is a an unknown constant vector, and the noise vector ε has the form $\sum_{i=1}^k \sigma_i Z_i$, where σ_i are unknown nonnegative coefficients and the Z_i are independent noise vectors with zero means and known covariance matrices. MINQUE accepts prior estimates of σ_i and produces new estimates by a calculation that is invariant to b .

In the present application the term Xb is absent; the noise is all there is. We treat only a simple two-parameter Gaussian noise model, in particular the phase of a clock with unknown levels of independent white FM (WFM) and random walk FM (RWFM) noises, sampled with period τ_0 . The mean drift rate is assumed to be zero. The data for MINQUE consist of the second increments of the phase samples, along with prior estimates of the noise levels. The first step of MINQUE is to normalize the unknown noise levels by the prior levels. The second step is to prewhiten the data according to the prior noise model. The last step is to apply the MINQUE criterion to calculate new estimates of the noise levels (Theorem 1) and their uncertainties (Theorem 2). We show examples using data from simulations and hydrogen maser measurements, and we see the effect of changing the prior noise levels. We also try feeding the estimates back into MINQUE repeatedly as new priors. The iterated estimates and their uncertainties appear to converge to reasonable limiting values independent of the original priors. The Appendix shows results from a Monte Carlo trial of the iterated estimates.

The original MINQUE calculation is a batch operation that does arithmetic on $N \times N$ matrices, where N is the number of data. After it was invented, statisticians discovered shortcuts [5–7] for carrying out the calculation in much less time and space. For the case treated here, the entire calculation can be carried out sequentially in $O(N)$ time and little space. A short summary of the algorithm is given below.

SETUP FOR A TWO-PARAMETER MINQUE

The data are modeled as a stationary process

$$z(n) = \sigma_1 Z_1(n) + \sigma_2 Z_2(n), \quad n = 1, \dots, N. \quad (1)$$

where $\sigma_i \geq 0$. The base processes $Z_i(n)$ are assumed to be independent Gaussian stationary moving-average (MA) processes of form

$$Z_i(n) = \theta_{i0} v_i(n) + \theta_{i1} v_i(n-1), \quad i = 1, 2, \quad (2)$$

where the θ_{ij} are known coefficients and the $v_i(n)$ are independent Gaussian random variables with mean zero and variance one.

SPECIAL CASE: WHITE FM + RANDOM WALK FM

Let a clock phase be modeled as $x(t) = x_1(t) + x_2(t)$, the sum of WFM and RWFM noises. The corresponding frequency spectrum is $S_y(f) = h_0 + h_{-2} f^{-2}$. We want to estimate h_0 and h_{-2} from $N+2$ samples $x(n\tau_0)$. Let $z(n)$ be their second increments,

$$z(n) = x(n\tau_0) - 2x((n+1)\tau_0) + x((n+2)\tau_0), \quad n = 1, \dots, N, \quad (3)$$

which form a stationary process. Unscaled dimensionless versions of the two components of $z(n)$ can be represented by the MA processes

$$\begin{aligned} Z_1(n) &= v_1(n) - v_1(n-1) \quad (\text{WFM}) \\ Z_2(n) &= v_2(n) + \beta v_2(n-1) \quad (\text{RWFM}) \end{aligned}$$

where $\beta = 2 - \sqrt{3}$. The correlation of $Z_2(n)$ and $Z_2(n-1)$ is 1/4; this is the crucial property of Z_2 that makes it equivalent to the second increment of an integrated continuous-time random walk. Now (1) holds, where

$$\sigma_1^2 = h_0 \frac{\tau_0}{2}, \quad \sigma_2^2 = h_{-2} \frac{4\pi^2 \tau_0^3}{3(1+\beta^2)}. \quad (4)$$

NORMALIZING BY PRIOR ESTIMATES

Returning to the general case, we want to estimate σ_1 and σ_2 from the data $z(1), \dots, z(N)$. The MINQUE method requires prior estimates $\tilde{\sigma}_i > 0$, which are used to normalize the unknown σ_i . Let

$$\gamma_i = \frac{\sigma_i}{\tilde{\sigma}_i}, \quad z_i(n) = \tilde{\sigma}_i Z_i(n), \quad \alpha_{ij} = \tilde{\sigma}_i \theta_{ij}. \quad (5)$$

Instead of (1) and (2), we work with the assumptions

$$z(n) = \gamma_1 z_1(n) + \gamma_2 z_2(n), \quad (6)$$

$$z_i(n) = \alpha_{i0} v_1(n) + \alpha_{i1} v_1(n-1). \quad (7)$$

The aim is to calculate estimates $\hat{\gamma}_i^2$ of γ_i^2 from the data $z(n)$. (It is possible for $\hat{\gamma}_i^2$ to come out negative.) Then σ_i^2 is estimated by

$$\hat{\sigma}_i^2 = \tilde{\sigma}_i^2 \hat{\gamma}_i^2. \quad (8)$$

In order to estimate and correct the overall scaling of the prior values $\tilde{\sigma}_i$, we give both γ_i an unknown prior value ζ that will be estimated from the data. Expectation and variance under the *prior assumptions* $\gamma_1 = \gamma_2 = \zeta$ are denoted by E_p and var_p .

PREWHITENING THE DATA

The data $z(n)$ will be transformed into new data $y(n)$ that are white under the prior assumptions. Write

$$z_i = [z_i(1) \quad \dots \quad z_i(N)]^T, \quad i=1,2, \quad (9)$$

$$z = \gamma_1 z_1 + \gamma_2 z_2. \quad (10)$$

Define the $N \times (N+1)$ Toeplitz matrix

$$L_i = \begin{bmatrix} \alpha_{i1} & \alpha_{i0} & & \\ & & \ddots & \\ & & & \alpha_{i1} & \alpha_{i0} \end{bmatrix} \quad (11)$$

and let $T = L_1 L_1^T + L_2 L_2^T$, which is assumed to be positive definite. By (7), (10), and the prior assumptions,

$$E z_i z_i^T = L_i L_i^T, \quad E_p z z^T = \zeta^2 T.$$

By Cholesky factorization, $T = L L^T$ for a nonsingular lower-triangular L , which we use to reduce z to an approximation of white noise. Let $y = L^{-1} z$, $y_i = L^{-1} z_i$. From (10),

$$y = \gamma_1 y_1 + \gamma_2 y_2, \quad (12)$$

and y_1, y_2 are independent mean-zero Gaussian vectors. Let

$$V_i = E y_i y_i^T. \quad (13)$$

Then

$$V_i = L^{-1} L_i L_i^T L^{-T} = M_i M_i^T, \quad (14)$$

where

$$M_i = L^{-1} L_i. \quad (15)$$

The true covariance matrix of y is

$$E y y^T = \gamma_1^2 V_1 + \gamma_2^2 V_2. \quad (16)$$

But, since $V_1 + V_2 = L^{-1} T L^{-T} = I$, y is white under the prior assumptions:

$$E_p y y^T = \zeta^2 I. \quad (17)$$

MINQUE ESTIMATORS

MATRIX PRELIMINARIES

1. Let A and B be real matrices of size $m \times n$. Regarded as vectors with mn components, their inner product is

$$\langle A, B \rangle = \sum_{i,j} a_{ij} b_{ij} = \text{tr} A B^T,$$

where tr is the trace operator. The Frobenius norm of a matrix A is

$$\|A\| = \sqrt{\langle A, A \rangle} = \sqrt{\sum_{i,j} a_{ij}^2} = \sqrt{\text{tr} A A^T}.$$

2. If A is symmetric and y is a column vector of correlated Gaussian random variables with $E y = 0$, $E y y^T = V = [v_{ij}]$, then

$$E y^T A y = \langle A, V \rangle = \text{tr } A V, \quad (18)$$

$$\text{var } y^T A y = 2 \langle A V, V A \rangle = 2 \text{tr } A V A V. \quad (19)$$

Equation (19) can be proved using Isserlis's formula [8],

$$\text{cov}(y_i y_j, y_k y_l) = v_{ik} v_{jl} + v_{il} v_{jk}.$$

MINQUE CRITERION

A MINQUE estimator of γ_i^2 ($i=1,2$) from the prewhitened data vector y of (12) is defined as a random variable $\hat{\gamma}_i^2 = y^T A_i y$, where A_i is a symmetric matrix chosen such that $\hat{\gamma}_i^2$ is unbiased for γ_i^2 and has minimum variance under the prior assumptions $\gamma_1 = \gamma_2 = \zeta$.

MINQUE SOLUTION

We shall see that the MINQUE estimators do not depend on ζ . One needs to know only the data vector y and the covariance matrices $V_i = E y_i y_i^T$ that come from the prewhitening calculation.

THEOREM 1. Assume that V_1, V_2 are linearly independent as $N \times N$ matrices. Let

$$S = \begin{bmatrix} \langle V_1, V_1 \rangle & \langle V_1, V_2 \rangle \\ \langle V_2, V_1 \rangle & \langle V_2, V_2 \rangle \end{bmatrix}, \quad q = \begin{bmatrix} y^T V_1 y \\ y^T V_2 y \end{bmatrix}. \quad (20)$$

The unique MINQUE estimators of γ_1^2, γ_2^2 are given by

$$\hat{\gamma}^2 := \begin{bmatrix} \hat{\gamma}_1^2 \\ \hat{\gamma}_2^2 \end{bmatrix} = S^{-1} q. \quad (21)$$

Proof. Let A_i be symmetric. By (18) with $A = A_i$ and V given by (16),

$$E y^T A_i y = \gamma_1^2 \langle A_i, V_1 \rangle + \gamma_2^2 \langle A_i, V_2 \rangle.$$

By (19) with $A = A_i$ and V given by (17) under the prior assumptions,

$$\text{var}_p y^T A_i y = 2 \zeta^4 \|A_i\|^2. \quad (22)$$

For $y^T A_i y$ to be unbiased for γ_i^2 whatever the true values of γ_1 and γ_2 , it is necessary and sufficient that

$$\langle A_i, V_1 \rangle = 1, \quad \langle A_i, V_2 \rangle = 0, \quad (23)$$

which is possible because of the linear independence assumption. According to the MINQUE criterion and (22), we are supposed to minimize the matrix norm of A_1 while keeping its matrix inner products with V_1 and V_2 fixed at 1 and 0. The minimizing A_1 is necessarily a matrix (an N^2 -vector) in the span of V_1 and V_2 ; any component orthogonal to that span would increase the norm. Thus, $A_1 = c_{11}V_1 + c_{12}V_2$ for some coefficients c_{11}, c_{12} . A similar argument for $y^T A_2 y$ gives $A_2 = c_{21}V_1 + c_{22}V_2$ for some c_{21}, c_{22} . Let $C = [c_{ij}]$. Altogether we have $\langle A_i, V_j \rangle = \delta_{ij}$ (Kronecker delta), and substituting for the A_i gives $CS = I$, $C = S^{-1}$. The MINQUE estimates of the γ_i^2 are then

$$\begin{aligned}\hat{\gamma}_1^2 &= y^T A_1 y = y^T (c_{11}V_1 + c_{12}V_2) y = c_{11}q_1 + c_{12}q_2 \\ \hat{\gamma}_2^2 &= y^T A_2 y = y^T (c_{21}V_1 + c_{22}V_2) y = c_{21}q_1 + c_{22}q_2.\end{aligned}$$

■

The original unknowns σ_i^2 are estimated by (8) from the prior estimates $\tilde{\sigma}_i^2$. As mentioned earlier, $\hat{\gamma}_i^2$ can be negative.

ESTIMATED MINQUE COVARIANCE

THEOREM 2. *Under the prior assumptions $\gamma_1 = \gamma_2 = \zeta$, the MINQUE estimator $\hat{\gamma}^2$ has covariance matrix*

$$R_{\gamma^2} = 2\zeta^4 S^{-1}.$$

Proof. Let A_i, S, C be as in the proof of Theorem 1. For an arbitrary 2-vector $u = [u_1 \ u_2]^T$,

$$u^T \hat{\gamma}^2 = u_1 y^T A_1 y + u_2 y^T A_2 y = y^T (u_1 A_1 + u_2 A_2) y$$

By (17) and (19), under the prior assumptions,

$$\text{var}_p u^T \hat{\gamma}^2 = 2\zeta^4 \|u_1 A_1 + u_2 A_2\|^2 = 2\zeta^4 \sum_{i,j} u_i u_j \langle A_i, A_j \rangle.$$

But

$$\langle A_i, A_j \rangle = \sum_{k,l} c_{ik} c_{jl} \langle V_k, V_l \rangle = \sum_{k,l} c_{ik} s_{kl} c_{jl} = (CSC)_{ij} = c_{ij}$$

since $C = S^{-1}$. Thus,

$$\text{var}_p u^T \hat{\gamma}^2 = u^T (2\zeta^4 S^{-1}) u$$

for any u . It follows that $2\zeta^4 S^{-1}$ is the prior covariance matrix of $\hat{\gamma}^2$. ■

Under the prior assumptions, $y^T y / \zeta^2$ is a χ_N^2 random variable, so let us estimate ζ^2 and R_{γ^2} by

$$\hat{\zeta}^2 = y^T y / N, \quad \hat{R}_{\gamma^2} = 2\hat{\zeta}^4 S^{-1}. \quad (24)$$

According to (8), we can estimate the standard deviation of $\hat{\sigma}_i^2$ from prior assumptions by

$$\text{std}_p \hat{\sigma}_i^2 = \tilde{\sigma}_i^2 \sqrt{\left(\hat{R}_{\gamma^2} \right)_{ii}}. \quad (25)$$

Neither the estimates (8) of σ_i^2 nor their estimated standard deviations (25) change when the prior estimates $\tilde{\sigma}_1$ and $\tilde{\sigma}_2$ are multiplied by the same constant. But the examples given below show that (25) is sensitive to multiplying them by different constants.

EXAMPLES

SIMULATED NOISE: WFM + RWFM

A simulation of $N=1000$ values of $z(n)$ as given by (3) was generated with the parameters $\tau_0=1$, $h_0=1$, $h_{-2}=1.900 \times 10^{-4}$. Results in the form of Allan deviation,

$$\sigma_y(\tau) = \sqrt{\frac{h_0}{2\tau} + \frac{h_{-2} 2\pi^2 \tau}{3}} \quad (26)$$

[9], are presented in Figures 1 and 2 for different prior values \tilde{h}_0 and \tilde{h}_{-2} mapped to $\tilde{\sigma}_1^2$ and $\tilde{\sigma}_2^2$ by (4). The black curve shows the Allan deviation for the true h_α . The figures also show the overlapped Allan deviation estimate for $\tau=2''$ with 68.3% confidence intervals calculated by the Stable software [10]. No confidence interval is calculated for the last point.

For Figure 1 we set prior estimates $\tilde{h}_0 = h_0/2$, $\tilde{h}_{-2} = 2h_{-2}$, that is, $\gamma_1^2 = 2$, $\gamma_2^2 = 1/2$. These give the prior Allan deviation shown by the red curve. The blue curve is the Allan deviation (26) from the estimates \hat{h}_α as mapped from the MINQUE estimates $\hat{\sigma}_i^2$ by (4). The dashed blue curves are the Allan deviations for $\hat{h}_\alpha + \text{std}_p \hat{h}_\alpha$ and $\hat{h}_\alpha - \text{std}_p \hat{h}_\alpha$, where the estimated standard deviation $\text{std}_p \hat{h}_\alpha$ is calculated from (25) and (4). The lower curve terminates when it goes negative, because $\text{std}_p \hat{h}_{-2} > \hat{h}_{-2}$.

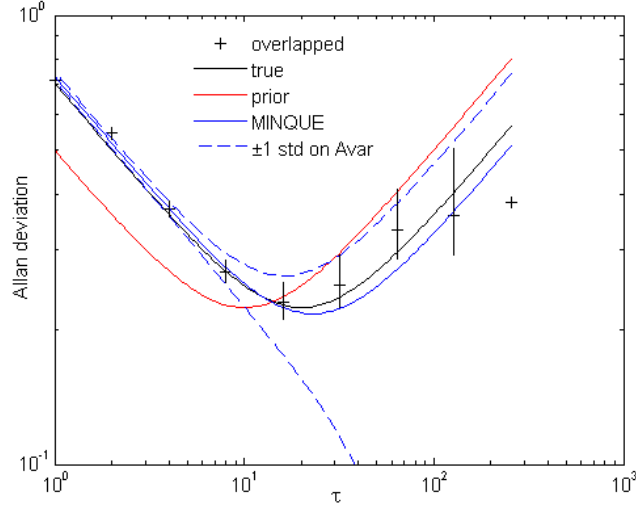


Figure 1. MINQUE estimate of simulated WFM + RWFM noise. The prior noise level was set to half the true level for WFM, twice for RWFM. The error bars show the overlapped Allan deviation estimate.

For Figure 2, we set $\tilde{h}_0 = 2h_0$, $\tilde{h}_{-2} = h_{-2}/2$. Now the $\pm 1 \text{ std}_p$ limits for the RWFM component seem to be too tight. For both cases, the WFM estimate \hat{h}_0 and its standard deviation are insensitive to the choice of prior estimates. The RWFM estimate \hat{h}_{-2} is somewhat more sensitive to the priors, but is still a good estimate of h_{-2} . Its estimated standard deviation is very sensitive to the priors, however.

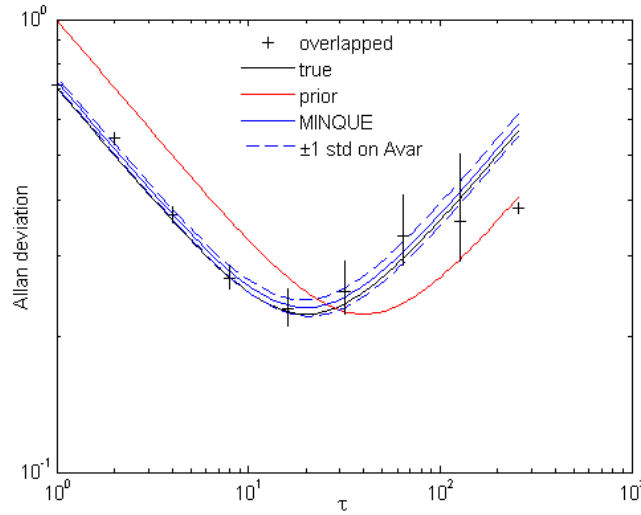


Figure 2. The ratios of prior levels to true levels are reversed.

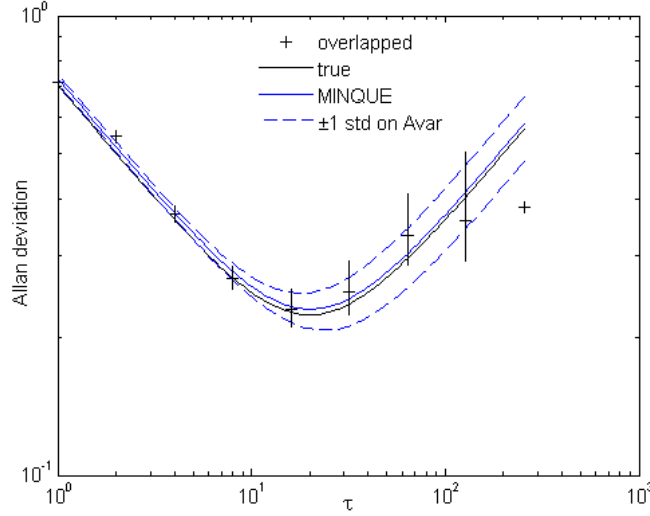


Figure 3. After 5 feedback iterations from either set of original priors.

ITERATED FEEDBACK OF ESTIMATES

Having calculated the MINQUE estimates, one can repeat the process with the same z data by using the \hat{h}_α in the role of the prior \tilde{h}_α and calculating new MINQUE estimates of h_α . This process can be repeated indefinitely as long as both \hat{h}_α are positive. For the examples that the author has tried, the estimated \hat{h}_α and standard deviations appear to converge to limits that are independent of the original priors. The estimated normalizing factor $\hat{\zeta}$ from (24) tends quickly to 1. For the simulated data, Figure 3 shows the result after 5 iterations. By luck, the limiting RWFM estimate is close to the true value. The standard deviation estimate looks reasonable in view of the Allan deviation confidence intervals. There are two questions: 1) Is the limiting \hat{h}_α unbiased? 2) How well does the limiting standard-deviation estimate represent the standard deviation of the limiting \hat{h}_α ? To answer these questions empirically, one can collect statistics on the limiting estimates over many simulated realizations of the clock noises (see the Appendix).

REAL PHASE NOISE: TWO HYDROGEN MASERS

Figure 4 shows overlapped Allan deviation with confidence intervals, the MINQUE estimate, and its estimated ± 1 std limits for a 2-week comparison of two hydrogen masers in JPL's Frequency Standards Laboratory. The phase data $x(t)$ were subsampled to 15 minutes from an original sample period of 1 second to get beyond the region of white and flicker phase. Their second increments (3) constitute the data for MINQUE. The overlapped Allan deviation estimate with error bars is also shown. The red curve is Allan deviation from the prior noise parameters $\tilde{h}_0 = 5 \times 10^{-27} \text{ s}$, $\tilde{h}_{-2} = 7.45 \times 10^{-36} \text{ s}^{-1}$, which were fit by eye from the Allan deviation estimates of the original data set. The prior WFM level seems too high for the subsampled data, and MINQUE adjusts it downward appropriately. Although RWFM looks like a poor fit for the long-term behavior, MINQUE chooses a reasonable estimate of the noise level. After five cycles of iterated feedback, the estimates do not change enough to make another plot worth showing.

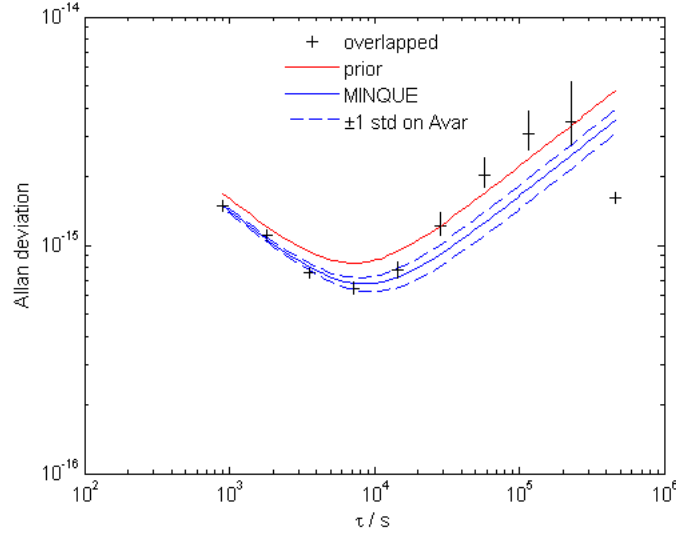


Figure 4. Applying MINQUE to the phase difference of two H-masers, assuming a noise model of WFM + RWFM.

SEQUENTIAL MINQUE ALGORITHM

If no attention is paid to the special structure of the matrices, the prewhitening calculation for N data takes $O(N^3)$ time and $O(N^2)$ space. The author was able to devise an iteration that calculates the S and q matrices of Theorem 1 from the z data and coefficients α_{ij} in $O(N)$ time and bounded space. For $n=1,2,\dots$, the algorithm receives $z(n)$ and updates a small structure of scalars, 2-vectors, and 2×2 matrices including $y(n)$, S , and q . The details are available from the author. For small values of n , equation (21) can give negative values of $\hat{\gamma}_i^2$; this is of no concern and the iteration can proceed.

CONCLUSIONS

Several techniques were introduced while implementing this case of Rao's MINQUE:

- Applying the MINQUE criterion after prewhitening the data according to the prior estimates of noise levels;
- Introducing and estimating a scaling factor ζ as the prior value of the normalized noise levels;
- Devising an $O(N)$ algorithm for the calculation (as also claimed in [6]);
- Estimating the noise level uncertainties;
- Feeding the estimated noise levels back into the algorithm as new prior levels.

The MINQUE method seems to work well for estimating the noise levels of the simple clock model of white FM plus random walk FM with no drift, giving lower RWFM uncertainty than overlapped Allan deviation does. The method requires prior estimates of the noise levels as inputs; for best results, it seems advisable to feed the output estimates back into the algorithm as new priors at least once or twice. The feedback experiments show empirically that the iteration converges to a fixed point not dependent on the

original priors. The fixed point constitutes another estimate of the noise levels. Properties of this estimate and its associated uncertainty matrix should be investigated theoretically and empirically (see the Appendix).

The sequential version of the algorithm might be simplified by using a time-invariant filter for the prewhitening operation. Perhaps the idea of applying the MINQUE criterion to prewhitened data could be extended to more complex situations with several noise components or several clocks.

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APPENDIX: EXPERIMENT ON ITERATED MINQUE

To investigate the properties of the fixed point of the MINQUE feedback iteration, 1000 independent realizations of 1000 values of WFM + RWFM noise were generated with the same noise levels h_α as before. For each realization, five feedback MINQUE iterations were run from randomized initial prior noise levels to get close to the fixed point. Statistics were collected on the noise level estimates \hat{h}_α and their estimated standard deviations. Figure 5 shows the results.

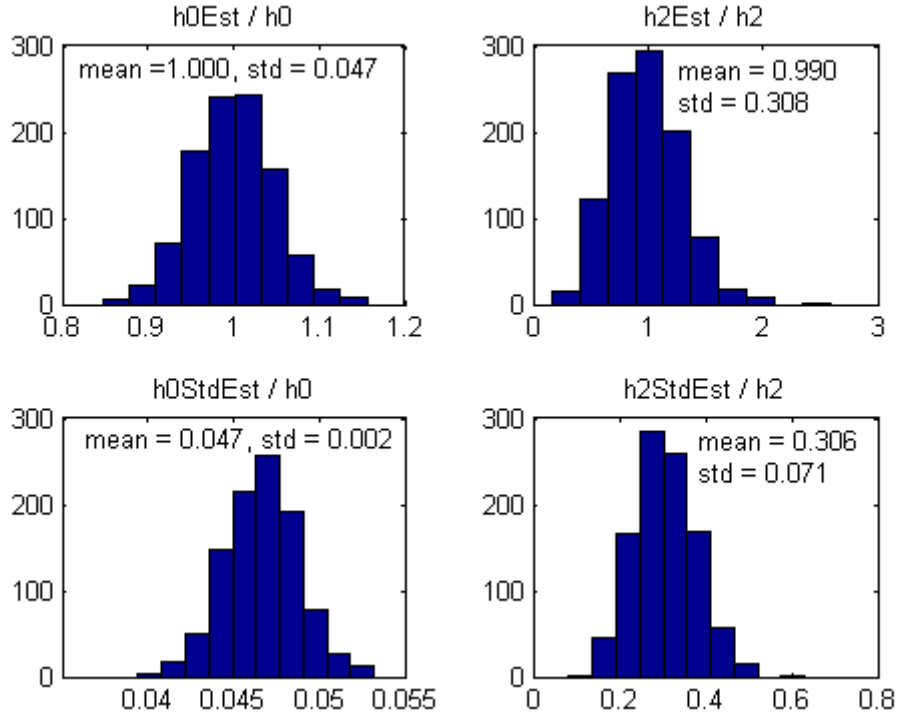


Figure 5. Experimental statistics of a case of iterated MINQUE.

The left-hand plots show the histograms of \hat{h}_0 (top plot) and its estimated standard deviation (bottom plot), normalized by the true value h_0 ; the right-hand plots show similar histograms for \hat{h}_{-2} . For both noise levels, the sample mean of \hat{h}_α is close to the true value, and the sample standard deviation of \hat{h}_α (std value in top plots) is close to the sample mean of the standard deviation estimate (mean value in bottom plots). The standard deviation estimate for \hat{h}_{-2} has a considerable spread, however.

Rao mentioned the possibility of MINQUE iteration [11]:

These estimates may then be substituted in (3.15), and the MINQUE procedure repeated. The whole process may be repeated several times, but then the property of unbiasedness is usually lost. It is possible that the estimates so obtained may have other interesting properties.

For the case investigated here, the iterated noise level estimates and their associated standard deviation estimates appear to be unbiased for practical purposes.